

Applying light microscopy and spectroscopic measurements, two phase transitions have been observed at $T_1 = 133$ K and at $T_2 = 106$ K, respectively. The transition at T_1 is interpreted as freezing of the disordered anions into two non-equivalent configurations [2]. By means of single crystal neutron diffraction the structural changes have been investigated as function of temperature [3]. Upon cooling the appearance of satellite reflections in the diffraction pattern at $T_1 = 133$ K was discovered. The positions of these satellite peaks and therefore the length of the \mathbf{q} -vector varies continuously with temperature. Therefore the structure is incommensurately modulated. Two other phase transitions have been observed at $T_2 = 107$ K and at $T_3 = 98$ K.

We have performed single crystal X-ray diffraction at beam line D3 of Hasylab (DESY, Hamburg) at $T = 100$ K. A first inspection of the data has shown, that the main reflections are regularly surrounded by satellite reflections up to second order. All observed peaks can be indexed in an hexagonal unit cell with $a = b = 8.441$ Å and $c = 15.732$ Å and the two \mathbf{q} -vectors $(\sigma, \sigma, 0)$ and $(-\sigma, 2\sigma, 0)$ with $\sigma = 0.0882$. We will present the results of the data analysis.

[1] Dubicki L., Ferguson J., Williamson B., *J. Phys. Chem.*, **1984**, 88, 4254. [2] Dubicki L., Ferguson J., Geue R.J., Sargeson A.M., *Chem. Phys. Lett.*, **1980**, 74, 393. [3] Larsen F.K., Jørgensen P., Grønbaek Hazell R., Lebech B., Thomas R., Geue R.J., Sargeson A.M., in *Molecular structure: Chemical reactivity and biological activity*, Stezowski *et al.* (ed.) IUCr, Oxford University Press **1988**.

Keywords: modulated structure; molecular compound; X-ray diffraction

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DRAWxtl 5.4 An Open-Source Program to Produce Crystal Structure Drawings. Martin Kroeker^a, Brian H. Toby^b, Larry W. Finger^c. ^a*Department of Inorganic Chemistry, University of Freiburg, Germany.* ^b*Advanced Light Source, ANL, Argonne, USA.* ^c*Retired from Carnegie Institution, Washington D.C, USA.*

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DRAWxtl is a versatile crystal structure drawing program that supports all the conventional drawing modes such as bonds, atomic spheres, thermal ellipsoids and coordination polyhedra of arbitrary complexity. Although it is mainly designed for the rendering of inorganic crystal structures, with import filters for CIF, CSD, Fullprof, GSAS and Shelx format, it is equally well suited for displaying results of LAPW calculations done with the popular VASP, WIEN2k and ELK/Exciting programs.

A significant new feature highlighted in our most recent publication[1] is its support for 3+1D to 3+3D modulated and composite crystal structures, including an interactive “walk through” the local structures that correspond to varying t values.

The upcoming 5.4 release, which should be available by the time of the conference, adds support for calculating and rendering cavity volumes and solvent-accessible surface areas and for displaying atomic basins as they result from

AIM calculations done with WIEN2k.

The program is freely available under the GPLv2 license from <http://www.lwfinger.net/drawxtl/> where we provide source code as well as pre-compiled versions for Linux, OS X and Windows.

[1] Finger L.W., Toby B.H., Kroeker, M., *J.Appl.Cryst.*, **2007**, 40, 188.

Keywords: computer programs; computer graphics; linux crystallographic computing

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RASTGUI - A Free Software Package for Reciprocal Space Mapping. Carsten Paulmann^a, Thomas Malcherek^a. ^a*Mineralogisch-Petrographisches Institut, Universität Hamburg, Hamburg, Germany.*
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Besides powerful X-ray sources and modern 2D-detectors on the experimental side, processing and visualisation of diffraction phenomena from disordered crystals require advanced software features covering non-integer indexed positions in reciprocal space (modulated structures, twinning) as well as a complete pixel-wise data processing to remap the irregular spaced experimental data to a regular grid. A range of command-line driven software tools for reciprocal space remapping were developed which include full four-circle support (Eulerian, Kappa) as well as advanced pixel-wise corrections (polarisation, scaling, background, phosphor incidence). The programs also provide internal binning options, definition of arbitrary planes of interest and most recently, masking options of obscured detector areas. Special versions are tailored to laboratory setups (Bruker-Nonius/Smart, Bruker-Nonius/KappaCCD) with fixed geometry whereas other versions aim for typical synchrotron hard- and software setups like MarCCD/XDS and also recently Mar345/XDS. With respect to the number of different experimental setups at synchrotron sources the diffractometer geometry is fully customisable. Additional tools provide enhanced numeric data processing features with special emphasis on synchrotron specific details (eg. primary beam scaling). However, the increasing number of different detectors, diffraction geometries as well as specific setup files and data processing control input files demanded the development of a common graphical user interface to guide less experienced users through the complete range of different data processing features and special advanced options. The interface was developed using the Qt4-library. Among the commonly supported hardware options, the users are able to define their specific experimental setup as well as program and data directories. Depending on the setup, the user interface provides special input masks for each software tool, generates specific input files and starts the basic command-line driven programs as background processes. Experienced users may still use the command-line versions to ease up the use of script files and cross-networking. Most recently, an OpenGL-based reciprocal space viewer was added which also features advanced options for a semi-automatic definition of the sample

orientation matrix and re-indexing of the corresponding reflection lists (Smart, XDS). The complete range of programs is freely available as Linux- or Windows-version upon contacting the authors.

Keywords: reciprocal space mapping; software; diffuse X-ray scattering

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Modeling of Decagonal Quasicrystals. Sofia Deloudi^a, Walter Steurer^a. ^aLaboratory of Crystallography, ETH Zurich, Switzerland.
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Quasiperiodic phases seem to naturally withstand the quantitative description we use for most periodic structures (for an overview of the field, see [1]). Providing good models is therefore crucial in order to understand quasiperiodic structures. They have to bring down the geometric principles of quasiperiodic structures to a few simple concepts, while closely resembling the real structures. Furthermore, they are useful tools for physicists in order to provide a good starting point for simulations. These demands can be fulfilled by the well-established technique of cluster-based modeling.

Among the axial quasicrystal structures, the system Al-Co-Ni is the best studied, but the discussion about the structures within this system is still ongoing. Its suitability as a model system is excellent because of several reasons. The phase diagram is well investigated and shows a wide range of modifications of the decagonal phase as a function of composition and temperature. Large single crystals can be easily grown, and electron-microscopic and surface-imaging methods can be used due to the short translation period along the tenfold axis.

In a previous work [2] we have presented a fundamental cluster with 20 Å diameter which makes it possible to model all decagonal phases in the system Al-Co-Ni (including the approximants) systematically, with small changes in the atomic structure.

We have now extended the modeling to the systems Al-Co-Cu and Al-Fe-Ni, showing that it is possible to derive all these complex phases from only one building principle. Furthermore, it was even possible with this approach to predict and explain atomic flip positions within the structures of all phases.

Here, we will concentrate on the discussion of geometrical aspects of the models for Al-based decagonal QCs with a four-layer periodicity, such as the generation of flip positions and superstructures, and we will discuss the agreement of our models with experiment.

[1] Steurer W., Deloudi S., *Acta Crystallogr. Sect. A: Found. Crystallogr.*, **2008**, 64, 1. [2] Deloudi S., Steurer W., *Philos. Mag.*, **2007**, 87(18-21), 2727.

Keywords: quasicrystal; decagonal; modeling

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For Some Commensurately Modulated Structure, Different Index Conditions Can See Different

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Layer stacking may allow alternative origins or orientations for adjacent layers. A different sequence may give a different origin or orientation of a structure, but different unit cells and space groups are also possible. When different sequences coexist we need to upgrade the refinement model, especially when the prototype layer adjusts for different layer sequences.

Crystals of Bi(SPh)₃ are a case in point. Reflections for k even, $h+k = 4N$ define a 1:1 disordered parent structure in space group $C2/c$, $\mathbf{a}_p = \frac{1}{2} \mathbf{a}$, $\mathbf{b}_p = \frac{1}{2} \mathbf{b}$, $\mathbf{c}_p = \mathbf{c}$ in which only the S are resolved. Disordered layers perpendicular to \mathbf{a}^* of $P2_1/c$ symmetry can only be ordered by doubling b to create a $Z = 4$ layer of $P2_1/c$ symmetry. The Bi is near a screw axis. Ordered stacking chooses between layer origins $\frac{1}{2} \mathbf{b}$ apart, implying 4 parameters, but 8 possible layer sequences after fixing the origin of the first layer. Four of these have $P2_1/n$ symmetry modulo $\mathbf{a}, \mathbf{b}, \mathbf{c}$, but different origins. The other 4 can be formed as linear combinations of the previous 4 and have $P2_1/n$ symmetry modulo $\frac{1}{2} \mathbf{a}, \mathbf{b}, \mathbf{c}$ (two origins) and $P-1$ modulo $\frac{1}{4}(\mathbf{a} \pm \mathbf{b}), \mathbf{b}, \mathbf{c}$ (two orientations). Observed intensity for reflections with k even, $h + k \neq 4N$ means the layers relax after ordering. The loss of $2/m$ diffraction symmetry for h odd, k odd reflections implies there is an unequally twinned triclinic component. Observation of reflections excluded by the ordered $P-1$ options means other component structures are present. Refinement of a twin of a prototype structure of $P2_1/n$ symmetry modulo $\mathbf{a}, \mathbf{b}, \mathbf{c}$ disordered over different origins is unsatisfactory. This refinement scales symmetrized components of the prototype structure and these scales vary with index condition. Excluding certain index conditions from refinement allows the remaining reflections to improve but then omitted reflections fit worse. The coexistence of different prototype structures is a necessary model extension.

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Keywords: problem structure; refinement; modulated structure

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Structures of Some 4,5-Dichlorophthalimide Derivatives. Orhan Büyükgüngör^a, Mustafa Odabaşoğlu^b. ^aOndokuz Mayıs University, Department of Physics, Samsun-Turkey. ^bPamukkale University, Chemistry Programme, Denizli-Turkey.
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Phthalimide derivatives have been gaining considerable interest since 1979, after recognized the hypolipidemic activity of N-substituted phthalimide derivatives [1]. Later on, researchers reported the antihyperlipidemic [2], hypolipidemic [3], anticonvulsant [4] activity and other interesting aspects [5] of phthalimide derivatives. In view